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APPENDIX B

H₂S Data Reduction

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1 Calculating Absorption of a Lossy Gas Using Q

Calculating microwave opacity from a weakly absorbing gas mixture using a resonator requires measuring the quality factor of that resonator which necessitates accurately determining the center frequency (f_o) and the half power bandwidth (Δf) of a noisy resonant line. The center frequency can be determined very accurately and varies very little over many measurements (a few kHz at GHz frequencies or a few hundredths of a percent). The greater source of error in estimating the Q of a resonator comes from the bandwidth measurements. The half power bandwidth is determined essentially by eye-fitting a curve over a noisy resonant line and measuring with a spectrum analyzer.

Assuming uncorrelated measurement error (an unbiased observer) the best estimation of the bandwidth is obviously the mean of many measurements. Therefore,

$$\Delta f \approx \frac{1}{N} \sum_{i=1}^N \Delta f_i \quad (1)$$

where Δf_i are the individual bandwidth measurements. To determine the accuracy of the measurements we calculate the sample variance,

$$S_N^2 = \frac{1}{N-1} \sum_{i=1}^N (\Delta f_i - \Delta f)^2 \quad (2)$$

and finally the variance of our estimation from the "true" bandwidth due to electrical noise,

$$\sigma_N^2 = \frac{t_\sigma^2}{N} S_N^2 \quad (3)$$

where t_σ is the "student-t" for the 1σ confidence level given a Gaussian distribution. Recall that the student-t is a distribution to characterize the confidence level of a finite sample set where the degrees of freedom are the number of samples. For ten measurements, $t_\sigma = 1.1$ [5, pp. 255, 260].

One can also calculate some figures of merit to determine the stationarity of the data [5, pp. 255-6]. Divide the ten measurements into two groups of five and calculate the sample variance (s_1^2, s_2^2) and mean (m_1, m_2) of each group where $s_1 > s_2$ and $m_1 > m_2$. We can define a figure of merit for stationarity of the variance as $F_o = 0.156s_1^2/s_2^2$. If $F_o < 1$ then the variance is likely to be stationary. For the mean, we define $t_o = 0.974(m_1 - m_2)/\sqrt{s_1^2 + s_2^2}$ as the figure of merit and if $t_o < 1$ then the mean is likely to be stationary. If either one of these conditions does not hold the measurement is not stationary and should be considered suspect.

There are also instrument errors which must be taken into consideration as well. These stem from the limited accuracy of the spectrum analyzer and are calculated as follows [2]:

$$\sigma_o \approx 10^{-5} f_o + 0.15 \text{RBW} + 0.05 \text{SPAN} + L_o + 250 \quad \text{Hz} \quad (4)$$

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$$\sigma_{\Delta} \approx 10^{-5} BW + 200N + 4L_{BW} \quad \text{Hz} \quad (5)$$

where σ_o is the standard deviation of the center frequency measurement due to the spectrum analyser accuracy, σ_{Δ} the standard deviation of the bandwidth measurement, RBW is the resolution bandwidth, L the least significant digit, BW the bandwidth and N the harmonic number (see tables 1 and 2).

Freq. band	S	X	K
RBW [Hz]	300	1000	30000
SPAN [kHz]	50	100	2000
N	1	2	4
L_o	10	100	1000
L_{BW}	10	100	1000

Table 1: Spectrum analyser parameters

	σ_o [kHz]	σ_{Δ} [Hz]
S	25	240
X	90	800
K	320	4815

Table 2: Instrument uncertainty for the frequency bands.

It is then possible to estimate the measured bandwidth and characterize its uncertainty. What we measure from a conventional spectrum analyzer, however, is not the true spectrum of the resonator but rather the convolution of the resonator spectrum and the sweep filter spectrum. If $Y(f)$ is the output, $X(f)$ the input and $H(f)$ the filter, then

$$Y(f) = H(f) * X(f). \quad (6)$$

In the time domain, we have $y(t) = h(t)x(t)$ where $y(t)$ is the inverse Fourier transform of $Y(f)$ and so on. Therefore, the signal spectrum is,

$$X(f) = \mathcal{F}[y(t)/h(t)] \quad (7)$$

where $\mathcal{F}[\cdot]$ denotes a Fourier Transform. If we assume a Gaussian filter and a Gaussian input then the actual signal bandwidth is simply

$$\Delta f_Q = \sqrt{\Delta f^2 - \text{RBW}^2} \quad (8)$$

where Δf_Q is the "true" half power bandwidth and Δf is the measured mean bandwidth. The Q of the resonator is then simply

$$Q = \frac{f_o}{\Delta f_Q}. \quad (9)$$

We will discuss the error in the next section.

To calculate the absorption recall that

$$\frac{\alpha}{\beta} = \sqrt{\frac{\sqrt{1 + (\epsilon''/\epsilon')^2} - 1}{\sqrt{1 + (\epsilon''/\epsilon')^2} + 1}} \quad (10)$$

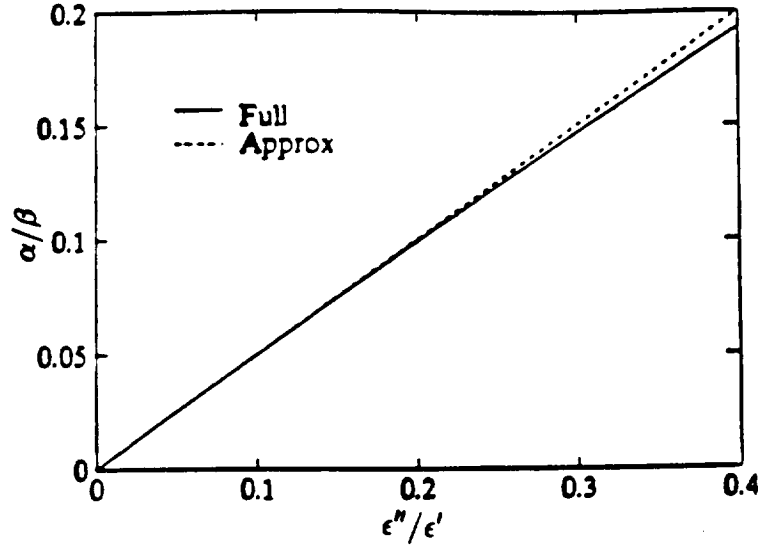


Figure 1: α/β vs. ϵ''/ϵ' for full expression (eq. 10) and approximation (eq. 11).

where $\beta = 2\pi/\lambda$ (with the gas present), α is the absorption and $\epsilon = \epsilon' - j\epsilon''$ the complex permittivity. Since $\epsilon'' \ll \epsilon'$ for gases in the microwave region this reduces to

$$\frac{\alpha}{\beta} \approx \frac{\epsilon''}{2\epsilon'}. \quad (11)$$

Note that this is field attenuation—to get power attenuation one must multiply this by 2.

The Q of a dielectric, Q_d , is given by

$$Q_d = \frac{1}{\tan \delta} = \frac{\omega \epsilon'}{\omega \epsilon'' + \sigma} \approx \frac{\epsilon'}{\epsilon''} \quad (12)$$

where the approximation holds for a gas at microwave frequencies. Therefore, we see that

$$\alpha \approx \frac{\beta}{2Q_d} = \frac{\pi}{\lambda} \frac{1}{Q_d}. \quad (13)$$

To determine Q_d we must examine the Q of a lossy, coupled resonator.

The measured quality factor of an evacuated resonator can be given by [1, p. 404]

$$\frac{1}{Q_{Tv}} = \frac{1}{Q_{Cv}} + \frac{1}{Q_{ev(1)}} + \frac{1}{Q_{ev(2)}} \quad (14)$$

and in the presence of a lossy gas

$$\frac{1}{Q_{Tg}} = \frac{1}{Q_{Cg}} + \frac{1}{Q_d} + \frac{1}{Q_{eg(1)}} + \frac{1}{Q_{eg(2)}} \quad (15)$$

where

- $Q_{Tv,g}$ = the total (measured) Q without and with the gas
- $Q_{Cv,g}$ = cavity Q without and with the gas
- $Q_{ev,g(1,2)}$ = external Q on both sides without and with the gas
- Q_d = Q of the gas.

Since a symmetrical cavity is used, assume that $Q_{eg,v(1)} = Q_{eg,v(2)} \doteq Q_{eg,v}$. Additionally [1, p. 404]

$$\frac{\sqrt{t_{g,v}}}{2Q_{Tg,v}} = \frac{1}{Q_{eg,v}} \quad (16)$$

where t_g and t_v are the transmissivities of the resonator at resonance with and without the gas respectively (assuming a lossless gas). Substituting into equations 14 and 15, subtracting and solving for $1/Q_d$ yields

$$\frac{1}{Q_d} = \frac{1 - \sqrt{t_g}}{Q_{Tg}} - \frac{1 - \sqrt{t_v}}{Q_{Tv}} + \frac{1}{Q_{Cv}} - \frac{1}{Q_{Cg}}. \quad (17)$$

Note that $Q_{Cv,g}$ takes conductivity losses and diffraction losses into account. The Q for finite conductivity, Q_σ , of a circular cavity varies as $1/\sqrt{f}$ [3, p. 352] we see therefore that

$$\frac{Q_{\sigma,v}}{Q_{\sigma,g}} = \sqrt{\frac{f_g}{f_v}} \approx 1. \quad (18)$$

For diffraction, likewise, the ratios of the Q's will be on the order of the ratios of the wavelengths and also equal to about 1, therefore $Q_{Cv} \approx Q_{Cg}$. Substituting these approximations into 17 yields

$$\frac{1}{Q_d} = \frac{1 - \sqrt{t_g}}{Q_{Tg}} - \frac{1 - \sqrt{t_v}}{Q_{Tv}}. \quad (19)$$

Recall that t_g assumes a lossless gas. Actually, the measured transmissivity, $t_{g,meas}$, equals $t_g e^{-\alpha d_{eff}}$ or

$$t_g = t_{g,meas} e^{\alpha d_{eff}} \quad (20)$$

where $d_{eff} = Q\lambda/2\pi$ is the effective path length of the resonator. We can then solve iteratively for the actual α .

We therefore see that

$$\alpha = \frac{\pi}{\lambda} \left(\frac{1 - \sqrt{t_g}}{Q_{Tg}} - \frac{1 - \sqrt{t_v}}{Q_{Tv}} \right) \quad \text{Nepers/m} \quad (21)$$

where λ is in meters. In dB, we can express α as

$$\alpha_{dB} = 8.686 \frac{\pi}{\lambda} \left(\frac{1 - \sqrt{t_g}}{Q_{Tg}} - \frac{1 - \sqrt{t_v}}{Q_{Tv}} \right) \quad \text{dB/m}. \quad (22)$$

The above analysis neglects the effects of dielectric loading [4]. Using an amount of lossless gas with the same refractivity value as the lossy gas in lieu of merely an evacuated resonator will remove the effects of the dielectric loading, provided you are far enough from the line center of the absorption line so that anomalous dispersion is not present.

2 Calculating the Error

Define a quantity

$$\xi = g(f_{og}, \Delta f_g, f_{ov}, \Delta f_v) = \frac{\gamma_g \Delta f_g}{f_{og}} - \frac{\gamma_v \Delta f_v}{f_{ov}} \quad (23)$$

where Δf_g and Δf_v are the loaded and unloaded half power bandwidths and f_{og} and f_{ov} are the loaded and unloaded center frequencies. We define this quantity since we wish to ignore the $1/\lambda$ dependence in front of α in the interest of symmetry. Then to first order

$$\begin{aligned} \delta \xi &= \frac{\partial g}{\partial f_{og}} \delta f_{og} + \frac{\partial g}{\partial \Delta f_g} \delta \Delta f_g + \frac{\partial g}{\partial f_{ov}} \delta f_{ov} + \frac{\partial g}{\partial \Delta f_v} \delta \Delta f_v \\ &= \frac{\gamma_v}{f_{ov}} \left[\frac{\Delta f_v \delta f_{ov}}{f_{ov}} - \delta \Delta f_v \right] - \frac{\gamma_g}{f_{og}} \left[\frac{\Delta f_g \delta f_{og}}{f_{og}} - \delta \Delta f_g \right] \\ &\equiv \Gamma_v - \Gamma_g. \end{aligned} \quad (24)$$

Note that this ignores variation in $\gamma = 1 - \sqrt{t}$.

Assume that $\langle \delta \xi \rangle = 0$ that is, we are dealing with zero-mean processes; therefore

$$\sigma_\xi^2 = \langle \delta \xi^2 \rangle = \langle \Gamma_v^2 \rangle + \langle \Gamma_g^2 \rangle - 2 \langle \Gamma_g \Gamma_v \rangle \quad (25)$$

where

$$\langle \Gamma_i^2 \rangle = \frac{\gamma_i^2}{f_{oi}^2} \left[\frac{\langle \delta f_{oi}^2 \rangle}{Q_i^2} + \langle \delta \Delta f_i^2 \rangle - \frac{2 \langle \delta f_{oi} \delta \Delta f_i \rangle}{Q_i} \right] \quad i = v, g \quad (26)$$

$$\langle \Gamma_v \Gamma_g \rangle = \frac{\gamma_v \gamma_g}{f_{og} f_{ov}} \left[\frac{\langle \delta f_{og} \delta f_{ov} \rangle}{Q_g Q_v} + \langle \delta \Delta f_g \delta \Delta f_v \rangle - \frac{\langle \delta f_{og} \delta \Delta f_v \rangle}{Q_g} - \frac{\langle \delta f_{ov} \delta \Delta f_g \rangle}{Q_v} \right] \quad (27)$$

$$Q_i = \frac{f_{oi}}{\Delta f_i} \quad (28)$$

The bandwidth variation consists of instrument accuracy and noise; i.e. $\delta \Delta f_i = \delta \Delta f_{SA} + \delta \Delta f_{Ni}$. Throughout, we will assume that electrical noise and the spectrum analyzer accuracy are uncorrelated. Since we have assumed zero-mean processes and uncorrelated accuracy/noise then

$$\langle \delta f_{oi}^2 \rangle = \sigma_o^2 \quad (29)$$

$$\langle \delta \Delta f_i^2 \rangle = \sigma_\Delta^2 + \sigma_{Ni}^2 \quad (30)$$

The uncertainty of the measured gas absorption, α , is then

$$\pm \frac{8.686\pi}{\lambda} \sigma_\xi \quad \text{dB/m} \quad (31)$$

where we have neglected the uncertainty in the measurement of λ . There are three cases that we will consider: the uncorrelated case, the "worst" correlation case and the "best" correlation case.

2.1 Uncorrelated Case

In the uncorrelated case, where naturally all variations are uncorrelated with one another, we find that

$$\langle \Gamma_i^2 \rangle = \frac{\gamma_i^2}{f_{oi}^2} \left[\frac{\sigma_o^2}{Q_i^2} + \sigma_\Delta^2 + \sigma_{Ni}^2 \right] \quad (32)$$

$$\langle \Gamma_g \Gamma_v \rangle = 0. \quad (33)$$

2.2 Worst Case

In the worst case scenario (the greatest error), $\delta f_v \delta \Delta f_g$ and $\delta f_g \delta \Delta f_v$ terms are completely correlated while the other terms are completely anti-correlated and, of course, the electrical noise terms are uncorrelated with the instrument accuracy terms. This yields

$$\langle \Gamma_i^2 \rangle = \frac{\gamma_i^2}{f_{oi}^2} \left[\frac{\sigma_o^2}{Q_i^2} + \sigma_\Delta^2 + \sigma_{Ni}^2 + \frac{2\sigma_o\sigma_\Delta}{Q_i} \right] \quad (34)$$

$$\langle \Gamma_v \Gamma_g \rangle = -\frac{\gamma_v \gamma_g}{f_{og} f_{ov}} \left[\frac{\sigma_o^2}{Q_g Q_v} + \sigma_\Delta^2 + \frac{\sigma_o\sigma_\Delta}{Q_g} + \frac{\sigma_o\sigma_\Delta}{Q_v} \right]. \quad (35)$$

This is the case typically used for the error, since a few small error terms have been neglected in this derivation.

2..3 Best Case

The best case scenario is the reverse of the worst case; that is $\delta f_v \delta \Delta f_g$ and $\delta f_g \delta \Delta f_v$ terms are completely anti-correlated while the other terms are completely correlated. This yields

$$\langle \Gamma_i^2 \rangle = \frac{\gamma_i^2}{f_{oi}^2} \left[\frac{\sigma_o^2}{Q_i^2} + \sigma_\Delta^2 + \sigma_{Ni}^2 - \frac{2\sigma_o\sigma_\Delta}{Q_i} \right] \quad (36)$$

$$\langle \Gamma_v \Gamma_g \rangle = \frac{\gamma_v \gamma_g}{f_{og} f_{ov}} \left[\frac{\sigma_o^2}{Q_g Q_v} + \sigma_\Delta^2 + \frac{\sigma_o\sigma_\Delta}{Q_g} + \frac{\sigma_o\sigma_\Delta}{Q_v} \right]. \quad (37)$$

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